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Using an Arbitrary Moment Predictor to Investigate the Optimal Choice of Prognostic Moments in Bulk Cloud Microphysics Schemes

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Key Points:

- A bin microphysics scheme is modified to act like a bulk microphysics scheme.
- The new scheme can predict arbitrary combinations of two or three moments of the hydrometeor size distribution.
- Box model tests show that standard configurations of two-moment schemes perform poorly for predicting some microphysical processes.

Abstract

Most bulk cloud microphysics schemes predict up to three standard properties of hydrometeor size distributions, namely, the mass mixing ratio, number concentration, and reflectivity factor in order of increasing scheme complexity. However, it is unclear whether this combination of properties is optimal for obtaining the best simulation of clouds and precipitation in models. In this study, a bin microphysics scheme has been modified to act like a bulk microphysics scheme. The new scheme can predict an arbitrary combination of two or three moments of the hydrometeor size distributions. As a first test of the arbitrary moment predictor (AMP), box model simulations of condensation, evaporation, and collision-coalescence are conducted for a variety of initial cloud droplet distributions and for a variety of configurations of AMP. The performance of AMP is assessed relative to the bin scheme from which it was built. The results show that no double- or triple-moment configuration of AMP can simultaneously minimize the error of all cloud droplet distribution moments. In general, predicting low-order moments helps to minimize errors in the cloud droplet number concentration, but predicting high-order moments tends to minimize errors in the cloud mass mixing ratio. The results have implications for which moments should be predicted by bulk microphysics schemes for the cloud droplet category.

Plain Language Summary

Countless cloud droplets with a variety of sizes exist in every cloud. Since cloud models cannot keep track of every individual droplet, most models instead predict quantities such as the total mass of cloud droplets and the total number of cloud droplets inside a model grid box. The values of these quantities dictate how fast clouds grow, how spatially extensive they are, and how well they reflect sunlight. In this study we explore whether the evolution of clouds could be improved if models instead predicted other properties of the cloud droplets, such as total surface area of all droplets or total diameter of all droplets. Our results show that improvements to current cloud models are likely possible.

1 Introduction

With improvements in computational speed and memory, atmospheric models are being designed with increasingly complex parameterizations to represent physical processes and systems such as the land surface, ocean, sub-grid turbulence, convection, and clouds. One of the more computationally expensive parameterizations in many contemporary models is the cloud microphysics parameterization. Traditionally, microphysics parameterizations predicted only the total mass mixing ratio (proportional to the 3rd moment of particle size distributions, or PSDs) of a limited number of cloud hydrometeor categories (e.g. Kessler 1969; Lin et al. 1983). Such schemes are known as single-moment schemes. It is becoming common for weather and climate models to predict both the mass mixing ratio and number concentration (0^{th} moment of PSDs) of each hydrometeor type (e.g. Meyers et al., 1997; Morrison et al., 2005; Seifert & Beheng, 2006; Thompson & Eidhammer, 2014). Although these double-moment schemes take longer to run and can require more assumptions, most studies have found that the increased complexity of the scheme leads to better predictions (Ekman, 2014; Igel et al., 2015 and references therein). Triple-moment schemes, which predict an additional third property of the cloud particle size distributions (Dawson et al., 2014; Milbrandt & Yau, 2005; Shipway & Hill, 2012), are currently primarily used for research applications and are not nearly as prevalent as single- and double-moment schemes. Most, if not all, triple-moment schemes have been designed to predict the radar reflectivity factor (6^{th} moment of PSDs). A review of bulk microphysics schemes was given recently by Khain et al. (2015). Finally, it should be noted that the proportionality of the 3^{rd} moment to mass and 6^{th} moment to reflectivity factor is only strictly valid for constant density spheres such as spherical liquid drops. The proportionality does not hold for most ice hydrometeors. Since the focus of this study will be on liquid, I will continue to use these physical interpretations of the 3^{rd} and 6^{th} moments.

The choice to predict the 3^{rd}, 0^{th}, and 6^{th} moments in cloud microphysics schemes has been made naturally. The 3^{rd} moment must be predicted in order to absolutely conserve water mass in any model. Mass conservation is a law of physics; however, no other such fundamental laws exist to guide our choice of which additional moments to predict. The 0^{th} moment, or number concentration, is an easy property to understand and formulate predictive equations for. The earliest double-moment schemes provide little or no justification for the choice to predict this property because it is such an obvious one to make (Koenig and Murray 1976; Ziegler 1985). Perhaps the best motivation is that number concentration is strongly associated with the nucleation of new cloud droplets and ice crystals. Another motivation is that the number concentration is conserved during condensation and provides a constraint on the PSD during that process. Therefore, there are strong, physically-based arguments to be made for predicting the 0^{th} moment. Nonetheless, for other processes, such as collision-coalescence, it is not obvious that the 0^{th} moment is logically a better quantity to predict than another moment of the distribution since number is not conserved when droplets collect one another. Finally, predicting the 6^{th} moment, or reflectivity factor, in triple-moment schemes is convenient for contrasting model output and radar observations, and for data assimilation, but is a choice that is harder to motivate based on physical considerations.

From a statistical standpoint, Morrison et al. (2019) find that knowledge of just the 0^{th} and 3^{rd} moments gives little constraint on higher order moments. They suggest that predicting a combination of high and low moments such as is done by triple-moment schemes may be best for reducing uncertainty in the simulations of all moments. Therefore, there may be more uncertainty in which two moments ought to be predicted in a double-moment scheme than in which three moments ought to be predicted in a triple-moment scheme.

There has been no systematic study to address the question of which moments to predict, which in retrospect, is somewhat surprising. Wacker and Lüpkes (2009) and Milbrandt and McTaggart-Cowan (2010) examined the problem for the case of sedimentation. Both studies find that the evolution of the moments in a precipitation shaft strongly depends on the predicted moments and the value of the shape parameter in the gamma probability distribution function. Predicting the 0^{th} and 3^{rd} moments yields the lowest average error of the 0^{th}-7^{th} moments only if the shape parameter is diagnosed based on current conditions. Predicting the 0^{th} and 8^{th} moment yields the lowest average error when the shape parameter is held constant (Milbrandt & McTaggart-Cowan, 2010), but unfortunately does not give mass conservation.

Sedimentation is a relatively simple process to examine since it is essentially a moment advection problem. The difficulty in examining the dependency of additional processes on predicted moments lies in developing bulk scheme equations for each moment. Kogan and Belochitski (2012) developed equations for the 0^{th}, 2^{nd}, 3^{rd}, 4^{th}, and 6^{th} moments for all major warm phase processes and Szyrmer et al. (2005) developed generic tendency equations for any moment for condensation and evaporation. In this study a different approach is taken. To avoid developing equations, a bin microphysics scheme is modified to behave like a bulk scheme. The modifications allow the bin scheme to be run as a “bulk-emulating” arbitrary moment predictor scheme. This arbitrary moment predictor scheme can be run with either a double- or triple-moment configuration and with any combination of moments predicted. By comparing its performance to the underlying bin scheme, the new scheme is used to make suggestions about the optimal choice of prognostic moments in bulk microphysics schemes for the cloud droplet category.

The development of the new scheme is described in Section 2, simulations are described in Section 3, results for double-moment configurations are discussed in Section 4 and for triple-moment configurations in Section 5.

2 Methods

2.1 Overview

The design of the Arbitrary Moment Predictor (AMP) microphysics scheme follows work first described in Igel and van den Heever (2017). Their work has been substantially expanded and the AMP scheme is described in detail here for the first time. A similar methodology was also adopted by Paukert et al. (2019). A flow chart is shown in Figure 1 to illustrate the process *for a single arbitrary hydrometeor category*. The basic approach is to initialize a grid box with a binned distribution of hydrometeors for each hydrometeor species that conforms to a gamma probability distribution function (PDF) based on the current values of predicted moments of each species. Next, the bin microphysics routines are run using this binned gamma PDF. At the end of the call to the bin microphysics routines, a user-defined set of moments (i.e. the arbitrary moments) of the hydrometeor distributions are calculated. In a box model, these moments are used to find new parameters of the gamma PDF for each species at the beginning of the next time step. In a full physics model, these moments would be passed back to the main model for use in other routines such as advection. Currently AMP can be configured as a double- or triple-moment scheme by changing the number of moments that are calculated at the end of the microphysics routines. The number of moments is not required to be the same for each species, but the 3rd moment is always predicted. It would be trivial to also allow it to act like a single-moment scheme, but that has not been done. At this time, cloud droplets and raindrops are the only two hydrometeor species included in AMP.

2.2 Technical Description

In this section, the technical development of the AMP scheme is described. The particular bin microphysics scheme that is used in this study is the Hebrew University Spectral Bin Model (SBM) (Khain et al., 2004). In principle any bin scheme may be used.

Like in most bulk schemes, the number distribution in AMP is assumed to conform to a gamma PDF. This number distribution is defined here as

$$n\left(D \vee N_0, \nu, D_n\right)=\frac{dN}{d\ln D}=\frac{N_0}{\Gamma\left(\nu\right)}\left(\frac{D}{D_n}\right)^{\nu} e^{\frac{-D}{D_n}}$$

(1)

where n is the probability size distribution of a hydrometeor category, N is the cumulative size distribution, D is the hydrometeor diameter, N_0 is the total number mixing ratio, ν is the shape parameter, and D_n is the scaling diameter (Walko et al. 1995). Note that (1) uses dN/dln$D$ rather than dN/dD. This choice is made for convenience because the SBM uses a mass-doubling set of bins. Since mass will always be conserved in AMP, and because the SBM solves for mass mixing ratio in each bin, it is useful to also define a mass distribution as

$$r\left(D \vee r_0, \nu, D_n\right)=\frac{\pi}{6}\rho_w D^3 n\left(D\right)=\frac{r_0}{\Gamma\left(\nu+3\right)}\left(\frac{D}{D_n}\right)^{\nu+3} e^{\frac{-D}{D_n}}$$

(2)

where $r_0 = \frac{\pi}{6}\rho_w N_0 D_n^3 \frac{\Gamma(\nu+3)}{\Gamma(\nu)}$ is the mass mixing ratio for a hydrometeor category and $m(D) = \frac{\pi}{6}\rho_w D^3$ is the mass of a single hydrometeor. Finally, the number distribution can be rewritten with r_0 rather than N_0:

$$n(D \vee r_0, \nu, D_n) = \frac{r_0}{m(D)\Gamma(\nu+3)}\left(\frac{D}{D_n}\right)^{\nu+3} e^{\frac{-D}{D_n}}$$

(3)

At the beginning of each call to AMP, the values of the parameter set r_0, ν, D_n for both cloud droplets and rain must be determined from the predicted moments. For double-moment configurations of AMP, r_0 and D_n are determined from the values of the predicted moments of each species and the value of ν is specified as a constant value. For triple-moment configurations, all three parameters, r_0, D_n, and ν are determined solely from the values of the predicted moments of each species. The procedure for determining the parameter values is described fully in the Appendix. In brief, binned distributions are inherently doubly truncated, which forces us to use iterative methods to find the parameter set that creates a binned gamma $n(D)$ with the appropriate moment values. The procedure is applied to each hydrometeor species separately. Note that as in standard bulk schemes, AMP splits the liquid hydrometeors into two categories: cloud droplets and raindrops. Specifically, drops with diameters of 80 μm or larger are considered rain drops.

It is important to mention that AMP is treated as an ideal bulk scheme. As such, it will not behave in the same way as any particular existing bulk scheme. Existing bulk schemes often take very different approaches to parameterizing some processes, most notably for example, collision-coalescence. Existing bulk schemes artificially separate this process into autoconversion and accretion, whereas bin schemes, and by extension AMP, makes no such artificial distinction. As such, this study cannot make any comments on the strengths or weaknesses of the parameterization of individual processes in existing bulk schemes. Rather, the idea here is to suppose that AMP is a perfect bulk scheme, that is, one with a perfect representation of process rates, and the only limitation in this otherwise perfect scheme is that distributions must conform to gamma PDFs. While existing bulk schemes do not have perfect parameterizations currently, it can be supposed that a perfect parameterization that does not rely on binned representations could be developed in the future. In this case, how well could this "perfect" bulk scheme do?

Inherently AMP assumes that the underlying bin scheme is perfect. This is the primary limitation of the study since problems with bin schemes are known to exist – for example, numerical diffusion across bins can lead to artificially wide distributions (see Morrison et al. (2018) for a recent summary of these problems). Regardless, they are built on the fundamental physical principles and equations that underly the three processes that are investigated in this study with a minimal number of simplifying assumptions. For this reason, bin schemes have been used as a benchmark against which to compare bulk schemes in many past studies (see Khain et al. 2015). Furthermore, developers of many bulk schemes have used bin schemes to parameterize individual processes, such as sedimentation, collision-coalescence, and droplet activation (Feingold et al., 1998; Morrison & Milbrandt, 2015; Saleeby & Cotton, 2004, 2008; Thompson & Eidhammer, 2014; Thompson et al., 2008).

In regards to the specific bin scheme being used in this study, the HUCM SBM, it is imperfect like any other bin scheme. It should be noted that the developers of this bin scheme have extensively studied the problem of artificial broadening and minimized it to the extent possible (Khain et al., 2004; Pinsky & Khain, 2002). Nonetheless, it is acknowledged that errors in the bin scheme associated with spectral broadening or any other source will impact the quantitative results of this study.

3 Box Model Simulations

This paper describes initial tests that have been done using AMP to understand which (arbitrary) moments of the cloud droplet size distribution should be predicted to minimize the errors in distribution moments during condensation, evaporation, and collision-coalescence. Each process has been simulated in isolation in a 0-D box. A suite of 280 initial conditions are designed to span a reasonable phase space for initial cloud water content, cloud droplet concentration, and the cloud droplet size distribution shape parameter. Specifically, initial cloud water content ranges from 1 to 5 g/kg in increments of 1 g/kg, cloud droplet concentration is doubled from 100 to 3200 mg^{-1}, and the shape parameter ranges from 1 to 15 in increments of 2. The ranges of cloud water content and cloud droplet concentration give initial mass mean cloud droplet diameters of 8.4 µm to 58 µm. 58 µm is typical of very large cloud droplets or small drizzle drops.

Simulations with each initial condition were conducted with several configurations of AMP. Double-moment configurations predicting the 3rd and 0th, 2nd, 4th, 6th, or 8th moments of the cloud droplet category were tested. The double-moment configurations will be designated as 2M-3X where X indicates the second predicted moment. For example, 2M-34 indicates the AMP configuration with the 3rd and 4th moments predicted. In all 2M tests, the shape parameter was held constant for the duration of the simulations. For triple-moment configurations, all combinations of two even-numbered moments plus the third moment were tested for the cloud droplet category. Triple-moment configurations will be denoted 3M-3XY where X is the first predicted moment and Y is the second.

In 2M configurations, the 0^{th} and 3^{rd} moments of rain were always predicted; in 3M configurations, the 6^{th} moment of rain was also predicted. Additional testing showed that the results were not highly sensitive to the configuration of the rain category (not shown). Although accretion of cloud droplets by rain is the dominant mechanism by which cloud is converted to rain, the insensitivity to the rain configuration in the collision-coalescence tests is consistent with the theoretical work of Seifert and Beheng (2001) who showed that accretion rates are primarily controlled by the total mass mixing ratios of cloud and rain.

Simulations are also run with just the HUCM bin scheme without any use of gamma PDFs. These bin simulations will be used to evaluate the AMP simulations.

Both the condensation and evaporation tests were run with temperature of 283 K and pressure of 1000 hPa. Evaporation tests used a relative humidity of 95% while condensation tests used a supersaturation of 0.5%. The temperature, pressure, and humidity of the box was held constant in time. Condensation tests were run for one minute. Such a short time was used since droplet distributions growing by condensation quickly become unrealistically narrow in the absence of distribution broadening mechanisms that occur naturally outside of box model simulations. Evaporation tests were run for thirty minutes to allow enough time for complete evaporation of the initial cloud water. Collision-coalescence tests were also run for thirty minutes; unsurprisingly, many initial conditions failed to produce precipitation in that time. All sets of initial conditions that did not produce rain with any AMP configuration or with the bin model were discarded.

Although only two or three moments were predicted in each AMP simulation, values of all moments (0^{th} – 9^{th}) were diagnosed and written to the output after each time step by integrating over the final size distribution produced by the parameterization routines.

4 Results Using AMP in Double-Moment Configurations

Results for each process are analyzed similarly. A percent error was calculated for each moment in each simulation by comparing its value to that in the corresponding bin simulation. The bin simulations are considered truth for the purposes of comparison. Absolute values of the percent errors are used. For each diagnosed moment, there are 280 percent error values from the 280 initial conditions for each AMP configuration.

4.1 Condensation

The 5^{th}, 25^{th}, 50^{th}, 75^{th}, and 95^{th} percentiles of the 280 percent error values associated with the condensation simulations are shown in Figure 2 for the

0^{th}, 3^{rd}, and 6^{th} moments diagnosed after one minute of condensation. Most impressively, the percent error of the 3^{rd} moment (mass) is almost always 1% or less, regardless of the combination of moments predicted (Figure 2b). Errors increase somewhat from 2M-30 to 2M-38, but ultimately all configurations accurately predict the evolution of mass during condensation.

The cloud droplet number concentration (0^{th} moment) should be conserved during condensation since new particles are not generated by condensation. Figure 2a shows that conservation of the 0^{th} moment is only achieved by explicitly predicting the 0^{th} moment. Otherwise, there is about a 10-20% median error after one minute of condensation regardless of the moments predicted. This is quite a rapid increase in error that is approximately linear in time; after five minutes, the median error is about 60-100% (not shown). The most immediate concern may be that errors in the number concentration would propagate to errors in the average cloud droplet diameter. Figure 3a shows error distributions for the ratio of the 1st moment to the 0^{th} moment (mean diameter) and 3b shows error distributions for the ratio of the 3^{rd} moment to the 2^{nd} moment (effective diameter). They show that the median errors for these two quantities are not nearly so different between 2M-30 and the other 2M configurations after one minute as they are for the number concentration. For cloud droplet effective diameter, the median errors are quite similar across all configurations (Fig. 3b) since it does not rely on the prediction of number concentration. Therefore, while a lack of conservation of the cloud droplet number concentration propagates to an error in the mean diameter, this error is relatively small compared to the original error in number concentration.

Perhaps unsurprisingly, median errors in the 6^{th} moment are minimized by explicitly predicting the 6^{th} moment (Fig. 2c). Nonetheless, apart from 2M-30, all combinations of predicted moments have values of the 95^{th} percentile error of only about 20%. This result indicates that these configurations all generally keep errors in cloud droplet reflectivity factor low. However, 2M-30 is the only configuration for which errors in the predicted cloud droplet number concentration are low. Therefore, there is no AMP configuration which allows us to simultaneously minimize the errors in all moments even for a relatively simple physical process like condensation.

4.2 Evaporation

The errors in the AMP simulations are evaluated as a function of time for evaporation. Since the time for complete evaporation depends on the initial conditions, the fraction of mass remaining in the bin simulation of each simulation set is used as a proxy metric for time. Median percent errors are shown as a function of this “time” in the top row and the median evolution of the normalized moments are shown in the bottom row of Figure 4. The moments have been normalized by their initial value.

Median errors are generally 20% or less for both the 0^{th} and 3^{rd} cloud droplet moments regardless of the AMP configuration (Fig. 4a-b). Errors tend to be larger toward the end of the simulation when most cloud mass has already evaporated. So, while the percent errors are larger, the absolute errors are in fact small.

Unlike for condensation, 2M-30 does not result in substantially lower errors in the predicted cloud droplet number concentration compared to other configurations (Fig. 4a). In fact, by the end of the evaporation process, 2M-30 has the highest errors of all configurations. Figure 4d indicates that the 2M-30 simulations have the most variability in the evolution of the number concentration and that these simulations tend to evaporate full droplets too slowly. Similar behavior was seen by Igel and van den Heever (2017b). Evaporation will naturally result in a size distribution with a non-zero number of droplets in the smallest size bin, i.e. a truncated left distribution tail that is difficult to capture with fixed size distribution functions. However, the truncated left tail will be less prominent in distributions of higher moments, and therefore it may be easier numerically to capture the evolution of the distribution with these higher moments. To investigate this problem, the binned distribution of cloud droplets at the end of the call to the bin microphysics routines during each AMP simulation was written to a file. Each distribution could then be compared to the idealized distribution that was initialized at the start of the subsequent time step. When the 0^{th} moment is predicted with AMP, fitting a PDF to a truncated size distribution usually results in a left tail that is too small. For example, in 70% (91%) of left-truncated distributions after the first timestep, the number concentration in the first bin of the re-initialized gamma distribution is ≥50% (≥10%) less than the predicted number concentration in the first bin at the end of the previous time step. If the bin scheme were to always produced perfect gamma distributions, then these two values would always be equal. These statistics indicate that undersized left tails are quite common in 2M-30 configurations of AMP during evaporation. An undersized left tail would cause too few droplets to be evaporated during each time step as is observed in Figure 4d.

The 2M-32 configuration seems to best predict the cloud mass evolution for the first half of evaporation while the other configurations perform similarly (Figure 4b). For the reflectivity factor, predicting higher moments clearly leads to reductions in the median error (Figure 4c). Interestingly, for evaporation, the error in the 6^{th} moment is minimized by predicting the 8^{th} moment during the latter half of evaporation, and not by predicting the 6^{th} moment. For evaporation, it is clearly seen that predicting a moment does not necessarily lead to the best simulation of that moment – predicting the 0^{th} moment does not minimize errors in the number concentration and predicting the 6^{th} moment does not always minimize errors in the reflectivity factor. Lower errors for reflectivity factor with 2M-36 rather than 2M-30 are in agreement with the results of Szyrmer et al. (2005) who examined steady-state evaporation in a rain shaft model.

4.3 Collision-Coalescence

The results of the collision-coalescence tests are shown in Figure 5 in the same way as for evaporation in Figure 4. Recall that although tests are only run for the configuration and initial conditions of the cloud droplet category, the rain category is active in all collision-coalescence simulations. Therefore, total liquid mass is constant during all simulations.

Errors in the cloud droplet reflectivity factor are about the same for each AMP cloud droplet configuration (Figure 5c). However, the errors for the cloud droplet number concentration (Figure 5a) and mass mixing ratio (Figure 5b) are distinctly different for each AMP configuration. Errors in the cloud droplet number concentration increase whereas errors in the cloud droplet mass mixing ratio decrease as higher moments are predicted. The magnitude of errors varies substantially among the AMP configurations; median errors in the mass mixing ratio are 10% or less during the entire evolution of the cloud droplet distribution for 2M-38 whereas they approach 100% at the end of the process for 2M-30 (Figure 5b). This result suggests that the evolution of cloud mass during the collision-coalescence process could potentially be substantially improved in current bulk schemes by predicting a higher moment. The cost though is that the evolution of the cloud droplet number concentration would deteriorate. Of the three processes examined, collision-coalescence provides the clearest example of how no single AMP configuration minimizes the errors of all cloud droplet moments simultaneously.

Collision-coalescence errors also clearly illustrate some shortcomings of assuming a gamma PDF for the cloud droplet size distribution. Nearly all AMP simulations convert cloud mass to rain too slowly (Fig. 5e). Since AMP and the bin scheme both use the same parameterization for collision-coalescence, this slowness must be due to the use of an assumed size distribution function. The failure of all AMP configurations to produce rain quickly enough likely arises because the initiation of rain from a collection of cloud droplets depends crucially on the production of a small number of larger droplets that reside in the right tail of the cloud droplet size distribution. Any microphysics scheme must be able to “remember” that these larger droplets exist since they are the ones that will collect the most additional cloud droplets in subsequent time steps and first grow to rain drop sizes. When low moments of the distribution are predicted, Figure 6 shows that AMP indeed fails to retain the largest cloud droplets with an assumed gamma PDF in 90% or more of simulations when at the same time the corresponding bin simulations show that rain production has begun. As a result, these AMP configurations produce rain much too slowly (Fig. 5e). AMP is much more likely to remember the few-but-important large cloud droplets if high moments of the cloud droplet distribution are predicted since higher moments give more weight to these larger droplets. Figure 6 shows that this is the case although a large majority of simulations in 2M-36 and 2M-38 still underestimate the right tail of the cloud droplet distribution during the earliest stages of rain production in the bin simulations. Interestingly, 2M-36 and 2M-38 convert cloud water to rain too slowly even though the calculated 6^{th} moment tends to be too large (Fig. 5f). This result seems to illustrate just how difficult it is for a bulk scheme to replicate the behavior of a bin scheme even when the process parameterization is identical.

4.4 Discussion

It is impossible to take the results for all three microphysical processes and determine which is the “best” combination of moments to predict for the cloud droplet distribution. First, doing so will require running 3D simulations of warm phase clouds which is beyond the scope of this paper but is planned for future work. Second, the answer to this question seems likely to be application specific. For example, one combination of moments may be best for predicting liquid water path, while another is best for predicting cloud albedo.

Nonetheless, some synthesis of the preceding tests is desirable. To do so, the median time-averaged absolute normalized errors of the 0^{th} - 6^{th} moments of the cloud droplet distributions in the AMP simulations have been calculated for each AMP configuration and for each process. These errors are additionally averaged over all processes (colored lines in Figure 7) and across the 0^{th} to 3^{rd} moments (black line) and 0^{th} to 6^{th} moments (gray line). The normalization is done with respect to the initial values of each moment in each simulation and all processes are given equal weight in the average. These summary quantities are similar to the one used by Milbrandt and McTaggart-Cowen (2010).

Figure 7 clearly shows that the process-ensemble errors in the 0^{th} to 2^{nd} moments of the cloud droplet distribution are minimized for 2M-32 or 2M-34 whereas errors in all higher order moments are minimized in 2M-36 or 2M-38. The inability of 2M configurations to simultaneously simulate low and high moments well was also found by Szyrmer et al. (2005). Unsurprisingly then, the average error in all cloud distribution moments (both 0^{th}-3^{rd} and 0^{th} – 6^{th}) is minimized by predicting a middling moment (Figure 7). Predicting the 3^{rd} and 4^{th} moments or 3^{rd} and 6^{th} moments seem optimal. Morrison et al (2019) speculated that this may be the case based on their analysis of the relationships between moments of rain drop size distributions.

5 Results Using AMP in Triple-Moment Configurations

Simulations with AMP in triple-moment configurations were also conducted as described in Section 3. Median time-averaged absolute normalized errors of the number, mass, and reflectivity factor of the cloud droplet distribution like those in Figure 7 are shown in Figures 8-11 for each process and for all processes averaged together. While a lot of information is contained in each figure, I will focus on the ‘x’s and ‘o’s in each panel which indicate the configurations with the highest and lowest errors, respectively, for each moment.

Overall, the results for the 3M tests are qualitatively similar to the 2M tests. Cloud mass is well predicted during condensation regardless of the combination of predicted moments (Fig. 8). Droplet number concentration during condensation is only conserved if the 0^{th} moment is predicted (Fig. 8a-d), and cloud reflectivity factor errors are usually low if the 6^{th} or 8^{th} moment is predicted (right half of Fig. 8). Overall, errors during condensation are minimized in the 3M-304 and 3M-306 configurations (Fig. 8b-c). 3M-306 is the typical combination of moments predicted by triple-moment bulk schemes. Errors are maximized in the 3M-368 configuration.

Errors for cloud mass in AMP during evaporation are generally low for all 3M configurations (Fig. 9). Errors in the droplet number concentration are highest when the 0^{th} moment is actually predicted (Fig. 9a-d) whereas errors in number are minimized when combinations of higher order moments are predicted (Fig. 9h). Again, this unusual result may stem from large departures of size distributions from the assumed gamma PDF shape. As it turns out, all moments have their highest error when the 0^{th} moment is predicted – 3M-308 for lower order moments (Fig. 9d) or 3M-302 for higher order moments (Fig. 9a). Errors in reflectivity factor also remain lowest when combinations of higher order moments are predicted (Fig. 9h-j). These results taken together mean that errors overall are minimized in 3M-346 (Fig. 9h).

Again, the errors during collision-coalescence in 3M configurations of AMP mirror behaviors of 2M configurations. Errors in the number concentration are strongly reduced in 3M configurations when the 0^{th} moment is predicted regardless of which other moment is also predicted (Fig. 10a-d). 2M-30 results in lower errors than any 3M configuration that doesn’t include the 0^{th} moment (not shown). This result serves to emphasize the importance of predicting the 0^{th} moment of the cloud droplet size distribution during collision-coalescence in order to minimize errors in the evolution of the number concentration. On the other hand, errors in the higher order moments (4^{th}-6^{th}) are lowest in 3M-368 when errors in lower order moments (0^{th}-2^{nd}) are maximized (Fig. 10j). Errors in both the cloud droplet number and mass concentrations are lowest in 3M-308 (Fig. 10d). Although this configuration also has the highest errors for the 5^{th} and 6^{th} moments, errors in the 5^{th} and 6^{th} moments are generally similar regardless of the AMP configuration and so the overall errors are minimized for 3M-308 again.

Overall, errors in 0^{th}-3^{rd} moments of the cloud droplet size distribution are each minimized in a different configuration (3M-302, 3M-304, 3M-306, and 3M-328, respectively; Fig. 11a-c, g), and errors in the 4^{th}-6^{th} moments are all minimized in a fifth configuration (3M-368; Fig. 11j). Like for the 2M cloud droplet configurations, no single 3M configuration minimizes the error in all moments simultaneously. Likewise, errors in each of the three processes are minimized by predicting a different combination of moments – 3M-304/3M-306 for condensation, 3M-346 for evaporation, and 3M-308 for collision-coalescence (Fig. 9b-c, Fig. 9h, Fig. 10d). Evaporation stands out as the only process for which errors were minimized when the predicted integer moments are all close. For the other two processes, the optimal configuration includes both high and low order moments. This result agrees with Morrison et al. (2019) as discussed in the introduction.

The preceding paragraph identifies seven configurations as “best” for predicting the cloud droplet category depending on the evaluation used. This result serves to highlight that it is impossible to design a bulk scheme that can perform well under all circumstances. When all errors for the 0^{th}-3^{rd} moments are averaged together, 3M-304 emerges as the configuration with the lowest error (Fig. 11b), whereas when the 0^{th}-6^{th} moments are averaged together it is 3M-306 (Fig. 11c), although the difference in error between 3M-304 and 3M-306 is slight for both averages. While this error metric is by no means perfect, this result is an encouraging one since existing triple-moment schemes typically predict the 0^{th}, 3^{rd}, and 6^{th} moments.

5 Conclusions

In this study, a flexible “bulk-emulating”, arbitrary moment predictor microphysics scheme has been developed by modifying a bin microphysics scheme. Moments of the size distribution are calculated at the end of one microphysical time step, used to find parameters of the gamma PDF, and used to initialize a binned distribution at the start of the next microphysical time step. Therefore, the arbitrary moment predictor and bin schemes have identical process parameterizations, but different representations of the hydrometeor size distributions. There are two motivations for developing this scheme. First, it allows an “apples-to-apples” comparison of bulk and bin schemes and gives us a way to understand the consequences of assuming a gamma PDF in bulk schemes. Second, the arbitrary moment predictor scheme can predict any combination of distribution moments. This capability allows us to investigate which combinations of predicted moments minimize the errors of a bulk scheme. As far as the author is aware, these are novel capabilities for a cloud microphysics scheme.

The arbitrary moment predictor microphysics scheme was run in several configurations of the cloud droplet category for many different initial conditions in a box model. Three processes were investigated – condensation, evaporation, and collision-coalescence. The evolution of the number concentration, mass mixing ratio, and reflectivity factor of the cloud droplet size distribution were compared to their evolution using a pure bin scheme with the same initial conditions. Based on these simulations, the following conclusions are drawn:

- No 2M or 3M cloud droplet configuration can simultaneously minimize the error of all cloud droplet distribution moments. This result is in agreement with the results of Szyrmer et al. (2005) and Milbrandt and McTaggart-Cowan (2010) for precipitating hydrometeors.
- Predicting a moment may or may not minimize the error of that moment. During condensation the error in the number concentration and reflectivity factor was minimized when the 0^{th} moment and 6^{th} moment were predicted, respectively in both 2M and 3M configurations. During evaporation, errors in the number concentration were instead maximized when the 0^{th} moment was predicted.
- Errors during collision-coalescence were higher than those for condensation and evaporation. Nearly all arbitrary moment predictor simulations produced rain too slowly. This result points to a fundamental limitation of assuming gamma PDFs.
- Double-moment bulk schemes predicting the 3^{rd} and 4^{th} or 3^{rd} and 6^{th} moments of the cloud droplet size distribution may have the potential to perform better than those predicting the standard combination of the 3^{rd} and 0^{th} moments.
- Current triple-moment bulk schemes may already be predicting the optimal combination of cloud droplet size distribution moments.

The last two conclusion points need to be confirmed by running AMP in a 3D model with all processes occurring simultaneously. Implementation of AMP in a 3D model will be done in the future to further investigate and substantiate these results. The current results will serve as a basis for interpreting the results obtained in a 3D model.

Finally, it is important to frame the conclusions drawn above. The suggestions made by AMP are very general and only apply strictly to what may be thought of as the ideal bulk scheme. Existing bulk schemes behave in non-ideal ways. Therefore, in practice, real-world bulk schemes may not actually perform best when predicting the moments suggested above. Rather, what our results show is that an ideal bulk scheme with physical parameterizations as good as those in the bin scheme will behave best with the predicted moments above. As we continue to improve bulk schemes with better physics, the results should become ever more relevant.

Acknowledgments, Samples, and Data

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Appendix

Here the procedure for determining the parameter values for $n(D)$ at the start of the microphysics routines is described. The variable first, second, and third predicted moments will be referred to as the Ist, IInd and IIIrd predicted moments, respectively. Note, for example, that the IInd predicted moment is not necessarily the 2nd moment of a PSD. The IInd predicted moment instead is the second predicted moment and can take on any value (i.e. it is arbitrary) except for the 3rd. In standard bulk microphysics schemes, the Ist predicted moment is the 3rd moment and the IInd predicted moment is the 0th moment.

To start, it is important to point out that there are two sets of moments in the AMP scheme. The first is the set of moments *predicted* by the bin scheme, ${}^{p}M_j$. The subscript j is the moment number. For example, ${}^{p}M_3$ is the Ist predicted moment and ${}^{p}M_0$ is the IInd predicted moment in standard double-moment bulk schemes. At the start of the microphysics routines, the predicted moments are used to find parameters of $n(D)$. Once $n(D)$ is known, any moment of $n(D)$, not just the Ist, IInd and IIIrd moments, may be calculated. This brings us to the second set of moments, which are those moments *diagnosed* from $n(D)$ and denoted by ${}^{d}M_j$. The goal at the start of each call to the microphysics routines is to find a set of parameters r_0, ν, D_n of $n(D)$ such that ${}^{p}M_j = {}^{d}M_j$ for each hydrometeor type. At the end of each call to the microphysics routines, the values of ${}^{p}M_j$ are updated by calculating the corresponding values of ${}^{d}M_j$.

Moments of a continuous distribution are calculated by integrating $n(D)$ multiplied by a power of D over all diameters from 0 to ∞. In the model, the distribution is discretized which requires us to know the discrete value of $d\ln D$, also known as the bin width (w). For the case of mass-doubling bins, w = ln(2)/3 for all bins. The moments ${}^{d}M_j$ are then calculated as

$$ {}^{d}M_j = \sum_{i=1}^{nbins} n\left(D_i\right) D_i^j w $$

(A1)

To solve for the parameter set, we first recognize that r_0 is independent of D_n and ν and that all moments are directly proportional to r_0. This means that we can initially choose an arbitrary, temporary value of r_0 that we will call r_{0temp} for use in calculating ${}^{d}M_j$ for all j. In that case ${}^{d}M_j/{}^{p}M_j$ is a constant for all values of j. Specifically,

$$\frac{{}^{d}M_j}{{}^{p}M_j}=\frac{r_{0temp}}{r_0} \tag{A2}$$

Once D_n and ν are calculated, r_0 can be solved for analytically using Eq. A2 and then values of ${}^{d}M_j$ can be recalculated with the updated (true) value of r_0 such that ${}^{p}M_j={}^{d}M_j$.

For complete gamma PDFs, equations exist to solve analytically for D_n and ν. However, binned distributions inherently represent doubly-truncated distributions that span from the smallest bin's diameter to the largest bin's diameter. Analytical solutions for D_n and ν do not exist for truncated, incomplete gamma PDFs. To solve for these two parameters, we instead use iterative routines to minimize the error of ${}^{d}M_j$ compared to ${}^{p}M_j$. Values of ${}^{d}M_j$ can be calculated at any point during the iterative procedure from the current guesses of the parameter values. The goal is to ensure that at the end of the iterative procedure that Eq. A2 is satisfied.

From Eq. A2 we can write

$$\frac{{}^{p}M_{II}}{{}^{p}M_3}=\frac{{}^{d}M_{II}}{{}^{d}M_3} \text{ and } \frac{{}^{p}M_{III}}{{}^{p}M_3}=\frac{{}^{d}M_{III}}{{}^{d}M_3}$$

or

$$1-\frac{{}^{p}M_{II}}{{}^{p}M_3}\frac{{}^{d}M_3}{{}^{d}M_{II}}=0 \text{ and } 1-\frac{{}^{p}M_{III}}{{}^{p}M_3}\frac{{}^{d}M_3}{{}^{d}M_{III}}=0 \tag{A3}$$

if the correct values of D_n and ν have been determined. If the correct values of D_n and ν have not been determined, then the left-hand sides of (A3) can be evaluated to quantify the error associated with the current values of D_n and ν. The Fortran Minpack hybrd1.f routines are used to iteratively minimize the absolute value of the LHSs of Eq. A3. The performance of this routine (and all iterative solvers) depends crucially on the first guess for the parameters. To determine a first guess, we use either the values of the parameters from the previous timestep, or we use look-up tables. The look-up tables are functions of $\frac{{}^{p}M_{II}}{{}^{p}M_3}$ and $\frac{{}^{p}M_{III}}{{}^{p}M_3}$. Once D_n and ν have been determined, Eq. A2 is used with ${}^{p}M_3$ to solve for r_0. These lookup tables were constructed in MATLAB by systematically creating binned distributions with 4 million combinations of D_n and ν, calculating values of $\frac{{}^{p}M_{II}}{{}^{p}M_3}$ and $\frac{{}^{p}M_{III}}{{}^{p}M_3}$, and inverting the data to make D_n and ν functions of $\frac{{}^{p}M_{II}}{{}^{p}M_3}$ and $\frac{{}^{p}M_{III}}{{}^{p}M_3}$ in the tables.

It is possible to predict values of ${}^{p}M_j$ for which no solution exists in both the double- and triple-moment configurations. In this case we ensure that ${}^{p}M_3 = {}^{d}M_3$, and additionally if possible that ${}^{p}M_{II} = {}^{d}M_{II}$ in the triple-moment configurations. Therefore, mass is always conserved by AMP. In this case, values of ${}^{p}M_j$ are updated by finding the change in the initial and final values of ${}^{d}M_j$ and adding it to ${}^{p}M_j$.

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Figure Captions

Figure 1. A flow chart depicting the steps taken in AMP to predict moments of one hydrometeor species.

Figure 2. Box and whisker plots of the percent errors of the AMP simulations relative to the BIN simulations after one minute of condensation for the a) 0^{th}, b) 3^{rd}, and c) 6^{th} moments of the cloud droplet distributions. Boxes show the 25^{th}, 50^{th}, and 75^{th} percentiles of the error distributions, and whiskers show the 5^{th} and 95^{th} percentiles. See the text for more details.

Figure 3. Like Figure 2 except for (a) cloud droplet mean diameter and (b) cloud droplet effective diameter.

Figure 4. Evolution of the median percent error (a-c) and median normalized moment values (d-f) during evaporation for the (a, d) 0^{th}, (b, e) 3^{rd}, and (c, f) 6^{th} moments of the cloud droplet size distribution. 25^{th} and 75^{th} percentile values are shown intermittently. In (d-f), the median evolution of the bin simulations is shown by the black dashed line. Note that the x-axes in all panels are defined such that the black dashed line in (e) is straight.

Figure 5. As in Figure 4 except for the collision-coalescence tests.

Figure 6. Fraction of 2M AMP simulations in each configuration that have too few droplets in the largest cloud droplet bin (the right tail of the cloud droplet size distribution) when the distribution is initialized as a gamma PDF at the start of a time step compared to the explicit size distribution from which the moments are calculated at the end of the previous time step. The fractions are shown as a function of the time in the corresponding bin simulations at which a given fraction of the cloud mass remains unconverted to rain water (as in Figure 5).

Figure 7. Median across 2M AMP simulations (average of all three processes) in each configuration of the time-averaged absolute normalized error of the 0^{th} through 6^{th} moments of the cloud droplet size distribution. The black and gray lines show the mean average absolute error of the 0^{th}-3^{rd} moments and 0^{th}-6^{th} moments, respectively. Circles indicate the configuration with the lowest average error for each line.

Figure 8. Median across all AMP condensation simulations in each 3M configuration of the time-averaged absolute normalized error of the 0^{th} through 6^{th} moments of the cloud droplet size distribution. The light and dark orange bars show the mean average absolute error of the 0^{th}-3^{rd} moments and 0^{th}-6^{th} moments, respectively. ‘x’s and ‘o’s indicate the configuration with the highest and lowest average error, respectively, for each set of bars with the same color. Errors in (a-d) for the 0^{th} moment are not shown and are generally about 10^{-10}.

Figure 9. As in Figure 8 except for the evaporation simulations.

Figure 10. As in Figure 8 except for the collision-coalescence simulations.

Figure 11. As in Figure 8 except for the average across all process simulations.